REPORT DOCUMENTATION PAGE

Form Approved OMB NO. 0704-0188

1. REPORT DATE (DD-MM-YYYY)	2. REPORT TYPE	3. DATES COVERED (From - To)
03-07-2017	Final Report	27-Jul-2016 - 26-Apr-2017

4. TITLE AND SUBTITLE
Final Report: Modeling Rate-Dependent Dissipation in Granular Solids via Continuum Thermodynamics

5a. CONTRACT NUMBER
W911NF-16-1-0439

5b. GRANT NUMBER

5c. PROGRAM ELEMENT NUMBER
611102

5d. PROJECT NUMBER

5e. TASK NUMBER

5f. WORK UNIT NUMBER

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8. PERFORMING ORGANIZATION REPORT NUMBER

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS (ES)
U.S. Army Research Office
P.O. Box 12211
Research Triangle Park, NC 27709-2211

10. SPONSOR/MONITOR'S ACRONYM(S)
ARO

11. SPONSOR/MONITOR'S REPORT NUMBER(S)
69517-EG-II.3

12. DISTRIBUTION AVAILIBILITY STATEMENT
Approved for Public Release; Distribution Unlimited

13. SUPPLEMENTARY NOTES
The views, opinions and/or findings contained in this report are those of the author(s) and should not contrued as an official Department of the Army position, policy or decision, unless so designated by other documentation.

14. ABSTRACT
This project has investigated the physical processes controlling energy dissipation in granular media during high-pressure compression and penetration. For this purpose, it has formulated and validated new hypotheses about the interplay between the energy loss through surface area creation in single grains and the energy consumption of packed systems undergoing simultaneous comminution, shear and volume change. Energy scaling hypotheses at both particle and assembly scale have been used to quantify the role of the strain rate on the dissipative capacity of

15. SUBJECT TERMS
Granular Materials, Particle Fracture, Constitutive Relations; Creep; Rate Dependence

16. SECURITY CLASSIFICATION OF: a. REPORT	b. ABSTRACT	c. THIS PAGE	17. LIMITATION OF ABSTRACT	15. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
UU	UU	UU	UU		Giuseppe Buscarnera
					19b. TELEPHONE NUMBER 847-/49-1588

Standard Form 298 (Rev 8/98)
Prescribed by ANSI Std. Z39.18

Report Title

Final Report: Modeling Rate-Dependent Dissipation in Granular Solids via Continuum Thermodynamics

ABSTRACT

This project has investigated the physical processes controlling energy dissipation in granular media during high-pressure compression and penetration. For this purpose, it has formulated and validated new hypotheses about the interplay between the energy loss through surface area creation in single grains and the energy consumption of packed systems undergoing simultaneous comminution, shear and volume change. Energy scaling hypotheses at both particle and assembly scale have been used to quantify the role of the strain rate on the dissipative capacity of a granular material. Such hypotheses have been tested via experiments conducted at both length scales. Furthermore, a rate-dependent continuum model for crushable materials based on such evidence has been formulated. Fundamental principles of fracture mechanics and continuum thermodynamics have been used to derive the model equations, while the resulting formulation has been tested through experimental evidence available in the literature, as well as against new tests conducted on both single grains and packed samples. The main outcome of this project is a new multi-scale simulation methodology able to characterize the dissipative properties of granular systems on the basis of easily measurable particle-scale characteristics such as grain size, shape, mineralogy and degree of polydispersity.

Enter List of papers submitted or published that acknowledge ARO support from the start of the project to the date of this printing. List the papers, including journal references, in the following categories:

(a) Papers published in peer-reviewed journals (N/A for none)

Received		Paper
02/24/2017	1	Yida Zhang, Giuseppe Buscarnera. A rate-dependent breakage model based on the kinetics of crack growth at the grain scale, Geotechnique, ( ): . doi: 1,025,266.00
07/03/2017	2	Changbum Sohn, Yida Zhang, Mehmet Cil, Giuseppe Buscarnera. Experimental assessment of continuum breakage models accounting for mechanical interactions at particle contacts, Granular Matter, ( ): . doi: 1,049,765.00
TOTAL:	**2**	

Number of Papers published in peer-reviewed journals:

(b) Papers published in non-peer-reviewed journals (N/A for none)

Received	Paper

TOTAL:

Number of Papers published in non peer-reviewed journals:

(c) Presentations

Number of Presentations: 0.00

Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received   Paper

TOTAL:

Number of Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received   Paper

TOTAL:

Number of Peer-Reviewed Conference Proceeding publications (other than abstracts):

(d) Manuscripts

Received   Paper

TOTAL:

Number of Manuscripts:

Books

Received   Book

TOTAL:

Received Book Chapter

TOTAL:

Patents Submitted

Patents Awarded

Awards

ASCE Arthur Casagrande Award

Graduate Students

NAME	PERCENT_SUPPORTED	DISCIPLINE
Changbum Sohn	33	Civil Engineering
FTE Equivalent:	**0.33**	
Total Number:	**1**	

Names of Post Doctorates

NAME	PERCENT_SUPPORTED
Ferdinando Marinelli	0.60
Mehmet Cil	0.15
Zhenhao Shi	0.08
FTE Equivalent:	**0.83**
Total Number:	**3**

Names of Faculty Supported

NAME	PERCENT_SUPPORTED	National Academy Member
Giuseppe Buscarnera	0.00	
FTE Equivalent:	**0.00**	
Total Number:	**1**	

Names of Under Graduate students supported

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Student Metrics
This section only applies to graduating undergraduates supported by this agreement in this reporting period

The number of undergraduates funded by this agreement who graduated during this period: 0.00
The number of undergraduates funded by this agreement who graduated during this period with a degree in science, mathematics, engineering, or technology fields:...... 0.00
The number of undergraduates funded by your agreement who graduated during this period and will continue to pursue a graduate or Ph.D. degree in science, mathematics, engineering, or technology fields:...... 0.00
Number of graduating undergraduates who achieved a 3.5 GPA to 4.0 (4.0 max scale):...... 0.00
Number of graduating undergraduates funded by a DoD funded Center of Excellence grant for Education, Research and Engineering:...... 0.00
The number of undergraduates funded by your agreement who graduated during this period and intend to work for the Department of Defense 0.00
The number of undergraduates funded by your agreement who graduated during this period and will receive scholarships or fellowships for further studies in science, mathematics, engineering or technology fields:...... 0.00

Names of Personnel receiving masters degrees

NAME

Total Number:

Names of personnel receiving PHDs

NAME

Total Number:

Names of other research staff

NAME	PERCENT_SUPPORTED

FTE Equivalent:
Total Number:

Sub Contractors (DD882)

Inventions (DD882)

Scientific Progress

Foreword

This 9-month STIR project involved two key activities: (i) the validation of scaling laws linking the energy to comminute a granular solid to the properties of its particles; (ii) the formulation of a rate-dependent continuum law capturing the interplay between grain-scale fracture kinetics and macroscale rate-sensitivity. The most important outcomes of the project are the collection of new data to bridge fracture processes at grain scale to the collective crushing of particle packings, as well as a new constitutive theory for granular continua capturing the interplay between global dissipation and material microstructure. The results of the project elucidate the role of the grain properties on the inelasticity of granular solids, thus setting a vision to simulate penetration and high-pressure impact via continuum laws relying on the physics of fracture. The following text describes the scientific advances derived from the project. Supplementary material including figures and equations is provided in a separate attachment.

Summary of the Key Results

The first set of experiments conducted in this project tested the role of particle shape and size on the crushing of granular materials. The mechanics of crushing was investigated through experimental and theoretical analyses at both particle and assembly scales. In particular, the tests involved particles of varying size (from 0.15 to 1.5mm) and two classes of granular solids (i.e., spherical glass beads or angular quartz sands). The results showed that shape and size are two critical factors affecting the energetics of grain crushing, as well as the macroscopic crushability of a packed sample. Particularly, the use of a range of contact models and fracture laws showed that both the energy storage prior to fracture and the mode of particle failure are controlled by the shape of the grains. The findings of the study are detailed by Sohn et al. (2017) and can be summarized as follows: (i) By calibrating different elastic contact models against the force-displacement curves for single particles it was shown that the mechanism of energy storage prior to fracture in spherical particles is well approximated by a Hertzian law, while conical contact laws are necessary to explain the trends measured in the presence of non-negligible particle angularity; (ii) Considerable size-dependence of the particle strength, as well as of the energy stored in single grains at the onset of fracture, was found in both classes of particles. While the size-dependent trends of highly angular sands were captured by a surface fracture law assuming failure initiation at edge cracks, a bulk fracture model reflecting particle split in proximity of the median plane was found to explain more satisfactorily the size-dependent properties of glass beads; (iii) The analysis of size-dependent properties at the macroscopic scale displayed trends similar to those measured at the grain scale (i.e., the effect of local size dependencies was preserved in the granular continuum). In particular, the grain size-dependence of both the energy threshold for macroscopic comminution and the yielding stress at the onset of collective crushing were explained successfully through bulk fracture laws (e.g., in case of glass bead samples) or surface fracture models (e.g., in case of angular sands). This finding underpins a linear scaling between local and global dissipation which can be used to reproduce the macroscopic response of granular solids. In addition, it motivates the use of advanced fracture laws to simulate non-stationary (i.e., time-evolving) intra-grain cracks causing rate-sensitive fragmentation. Supplementary figures documenting the above investigation are provided in the attached documentation (Figures 1 to 7).

From a theoretical standpoint, the project has generated a new rate-dependent continuum breakage model inspired by the thermodynamics of subcritical crack propagation. One of the goals of the investigation was to explain the link between local grain fracture and comminution for the case of non-stationary cracks. To accomplish this, fracture kinetic theories were recast in the framework of thermodynamics with internal variables. This led to the identification of an additional energy dissipation term which (i) augments the loss of energy by surface area creation and (ii) generates rate-sensitivity through a non-homogeneous dependence on the crack growth rate. The power law coefficient of such higher-order function was found to depend on the well-known stress-corrosion index of brittle solids. Hence, by assuming that the rate effects of granular specimens under high pressures are controlled by the subcritical growth of cracks in individual particles, a new form of breakage dissipation has been proposed by incorporating the same degree of non-linearity valid for intra-grain cracks. Such hypothesis led to a continuum law in which the rate of delayed comminution is controlled once again by the stress corrosion index of the grain-forming solid. A rate-dependent continuum model was finally formulated by coupling the breakage dissipation with frictional shearing and plastic volume change. The resulting model was validated against a wide range of data for sands subjected to oedometric and triaxial compression. The analyses showed that the model exhibits an excellent performance in capturing complex patterns of response, including strain-rate sensitivity, creep histories, stress relaxation patterns and nonisotach viscous behaviour. All such features could be reproduced only by using a degree of nonlinearity of the viscous functions compatible with the values of corrosion index reported in the literature for quartz, silica and other rock-forming minerals. As a result, these findings validate the hypotheses about the role of subcritical crack growth on the macroscopic manifestation of rate-dependent crushing. The formulation of the theory, as well as the performance of the continuum model based on it, are detailed in Zhang and Buscarnera (2017). Supplementary figures describing the key hypotheses and results are provided in the attached documentation (Figures 8 to 11).

To provide further evidence about the link between delayed grain fracture and rate-dependent comminution, this project also conceived new experiments tracking the evolution of the system polydispersity for different stress states and packing conditions. While the analysis of the results and the consequent stage of model verification are not yet complete, some of the main conclusions that emerged from the experiments are summarized hereafter. In addition, supplementary figures are provided in the attached documentation (Figures 12 to 15). First, different quartz sands of varying mean grain size have been tested at constant rates of deformation to capture the evolution of the degree of polydispersity. Then, the accumulation of compaction over time under fixed stress states was monitored to assess the dependence between the viscous properties of the continuum on the size of the particles. These tests have been repeated multiple times to track the evolution of the grain size distribution. This step was crucial to assess the hypothesized link between the rate of breakage growth and the elastic energy stored in the continuum. The collected data enabled the quantification of the stress corrosion index controlling the rate-dependence of the continuum. Most importantly, it allowed the identification of the scaling relation between the times of failure of single particles and the timescale of delayed comminution. These results will constitute the basis of an additional journal publication currently in preparation, which will provide a robust reference to elucidate the connection between delayed processes at grain and continuum scales.

References

Sohn, C., Zhang, Y.D., Cil. M., Buscarnera, G. (2017). Experimental assessment of continuum breakage models accounting for mechanical interactions at particle contacts. To appear in Granular Matter.

Zhang, Y.D., Buscarnera, G. (2017). A rate-dependent breakage model based on the kinetics of crack growth at the grain scale. Géotechnique; http://dx.doi.org/10.1680/jgeot.16.P.181.

Technology Transfer

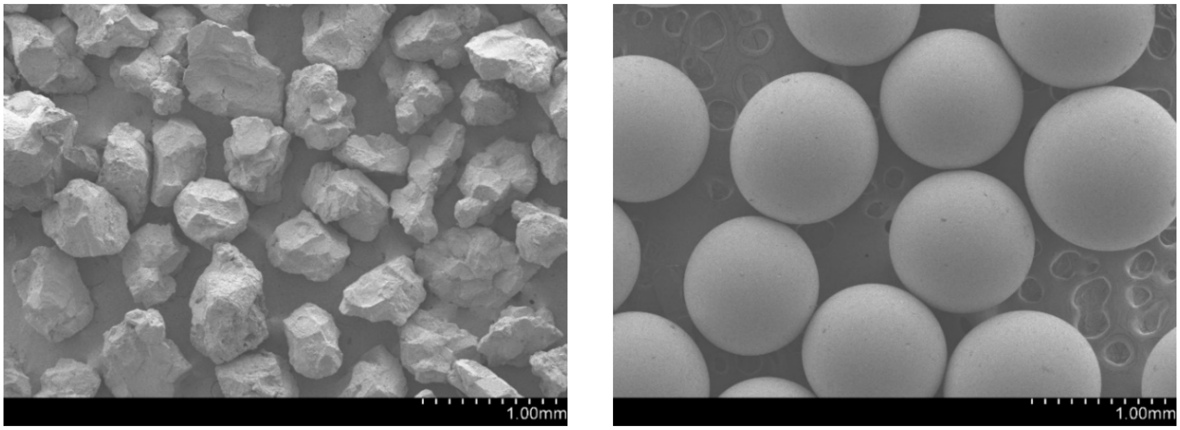


Figure 1. SEM images of the two classes of granular materials tested in this project (a) angular Q-ROK#1 sands (average diameter d_p = 0.350 mm); (b) well-rounded large glass beads (average diameter d_p = 1.132 mm). Particles of the same class with different size exhibit similar shape characteristics.

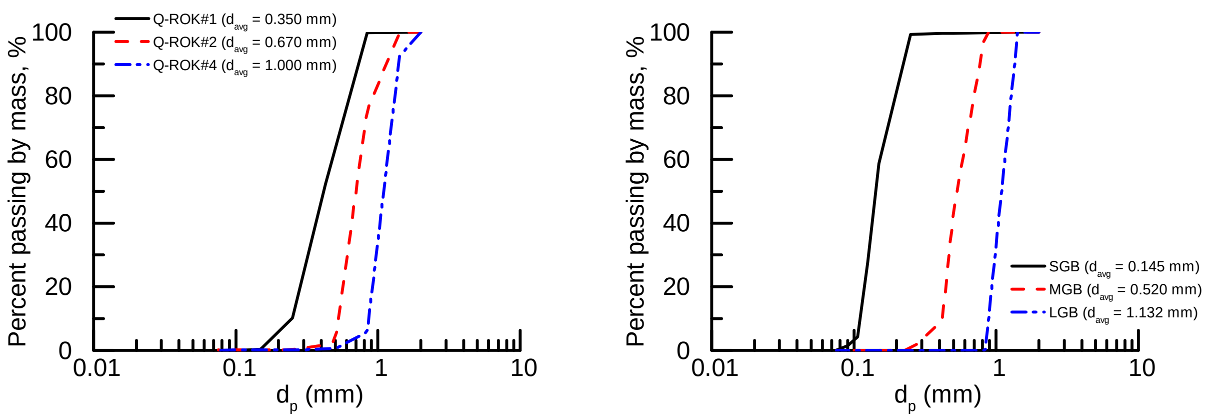


Figure 2. Grain size distributions of the granular media tested in this study: (a) Q-ROK sands; (b) glass beads. All the gradation data were obtained via standard sieve analyses.

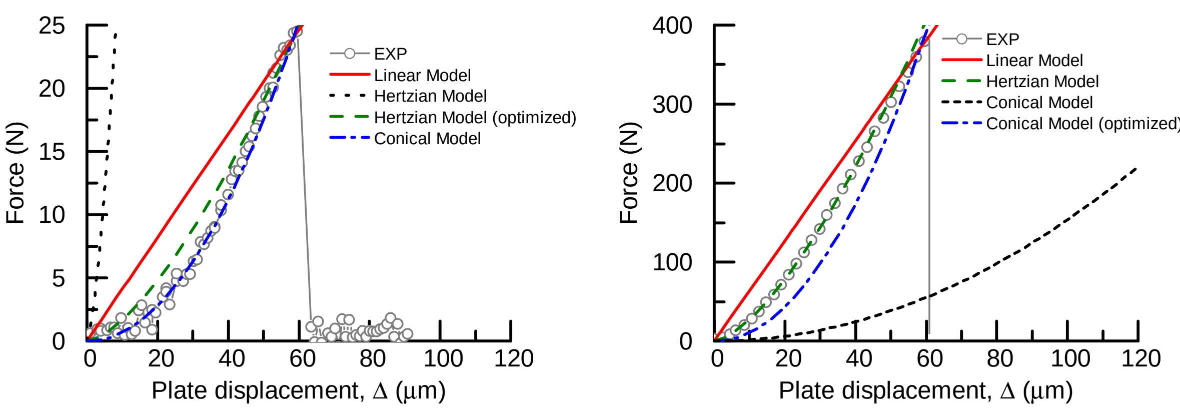


Figure 3. Examples of crushing tests on individual particles: (a) Q-ROK grains (d_p = 1.07 mm); (b) glass beads (d_p = 1.09 mm). Comparisons with model results are based on calibrated contact parameters specific for the chosen curves.

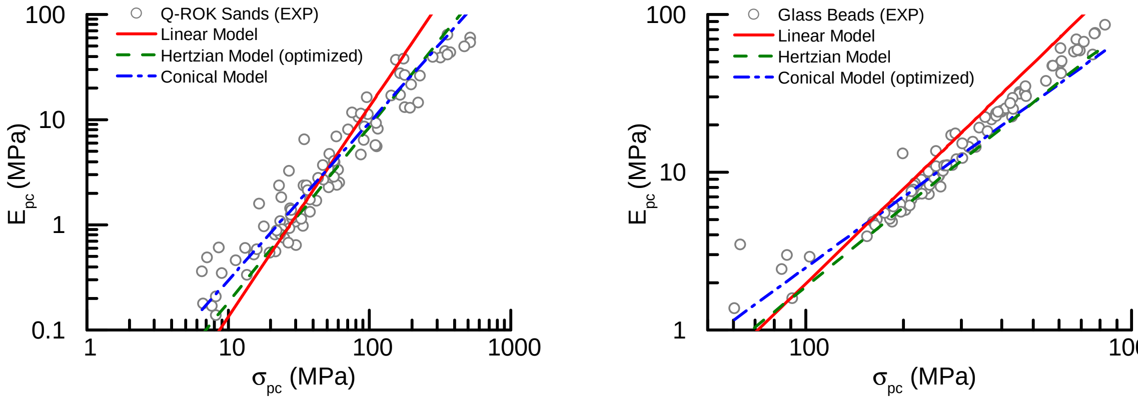


Figure 4. Energy-strength relationship for (a) Q-ROK sand grains and (b) glass beads. Trend lines indicate calibrated model predictions based on different contact models. The parameters used for the trend lines derive from an averaging of results obtained for 30 individual crushing experiments on randomly selected particles from each of the six batches of granular materials depicted in Figure 2.

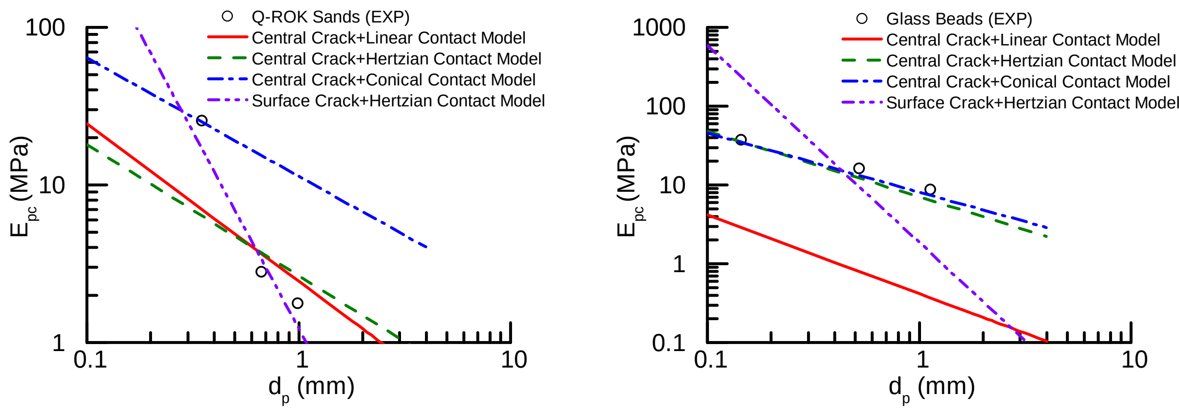


Figure 5. Values of energy released at the onset of fracture (E_{pc}) as a function of the particle diameter for (a) Q-ROK sand particles and (b) glass beads, along with predictions from four combinations of contact laws and fracture models.

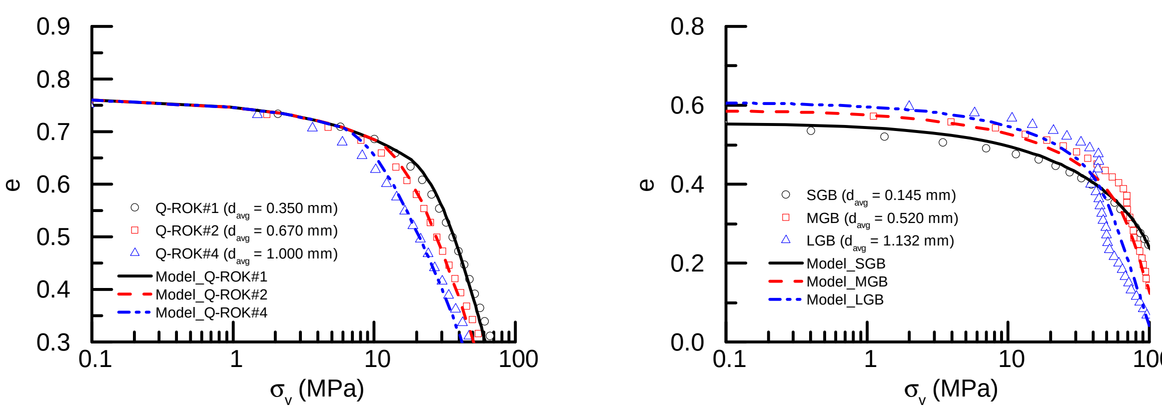


Figure 6. Results of oedometric compression tests and corresponding continuum model simulations for: (a) Q-ROK sands and (b) glass beads. To ensure consistent comparisons, all tests were run starting from the densest state of each of the tested materials.

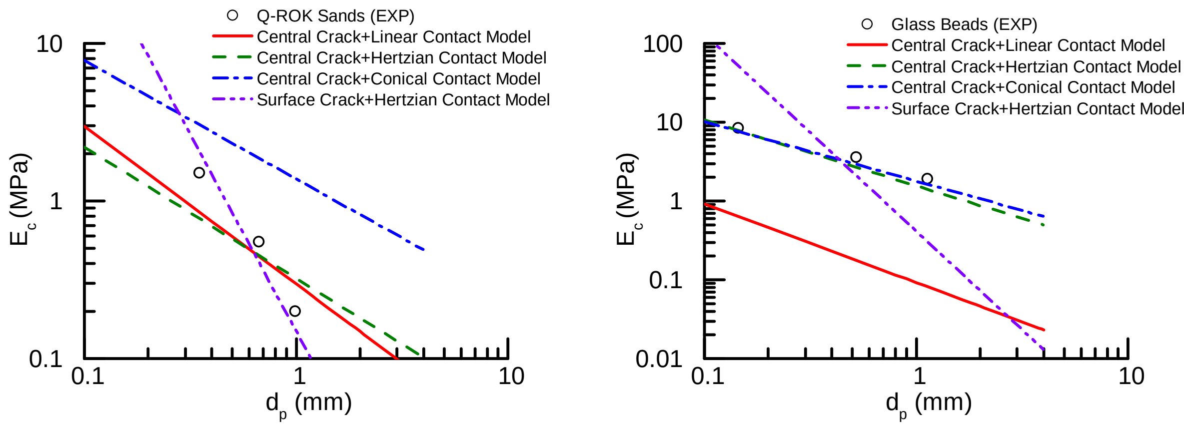
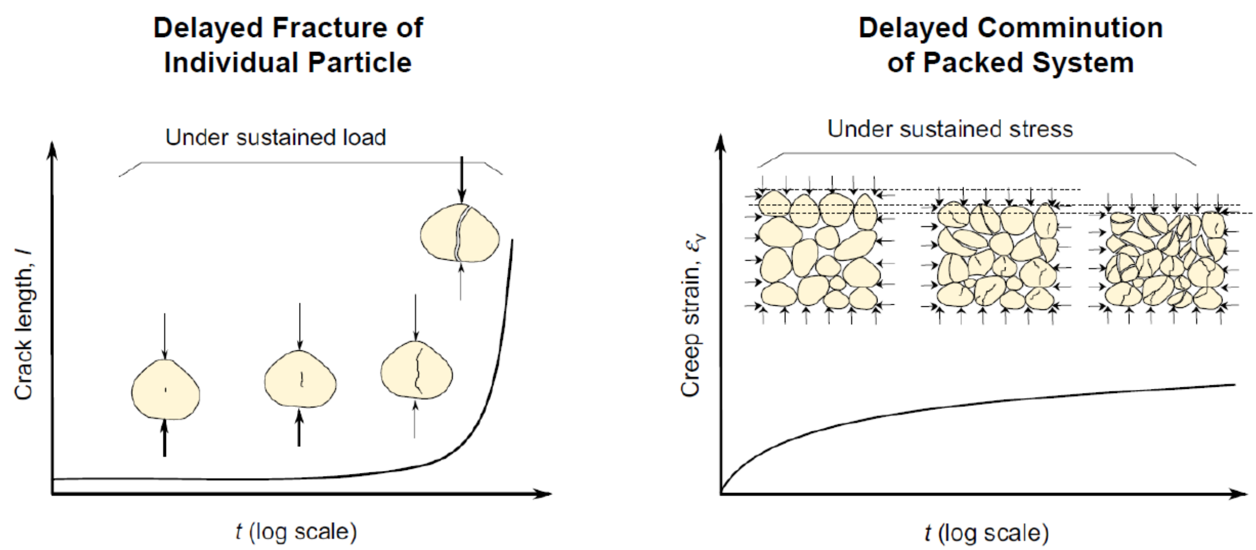


Figure 7. Critical Breakage Energy, E_c, at the continuum scale obtained for each tested granular packing. The energy threshold for collective comminution is plotted as a function of the particle diameter for (a) Q-ROK sand and (b) glass beads. The performance of four combinations of contact and fracture models is also shown. The results exhibit the same size-dependent trends observed at the grain scale (Figure 5).



$$\Phi(\dot{l}) = 2\gamma\dot{l}\left(1+\left(\frac{\dot{l}}{\dot{l}_0}\right)^{2/n}\right) \geq 0$$

$$\Phi(B,\dot{B}) = \frac{E_c\dot{B}}{(1-B)^2}\left(1+\left(\frac{\dot{B}}{\dot{B}_0}\right)^{2/n}\right)$$

Figure 8. Schematic representation of the thermodynamic analogy between the delayed fracture of individual grains and the delayed comminution of packed granular systems. The dissipation equation defined for individual fracture processes (left side of the schematic diagram) is designed to recover a power law kinetics. The factor n appearing in its expression is commonly referred to as *corrosion coefficient*. The terms outside the parentheses reflect the energy dissipation due to crack growth in rate-independent fracture. The dissipation equation used at the scale of a granular continuum has a similar mathematical form (right side of the schematic diagram). The terms outside the parentheses reflect the energy loss due to rate-independent comminution. They are augmented by a multiplicative factor having the same structure of that seen at the grain scale (and, hence, based on the same corrosion coefficient), but in which the Breakage growth rate replaces the crack extension velocity as the primary inelastic internal variable.

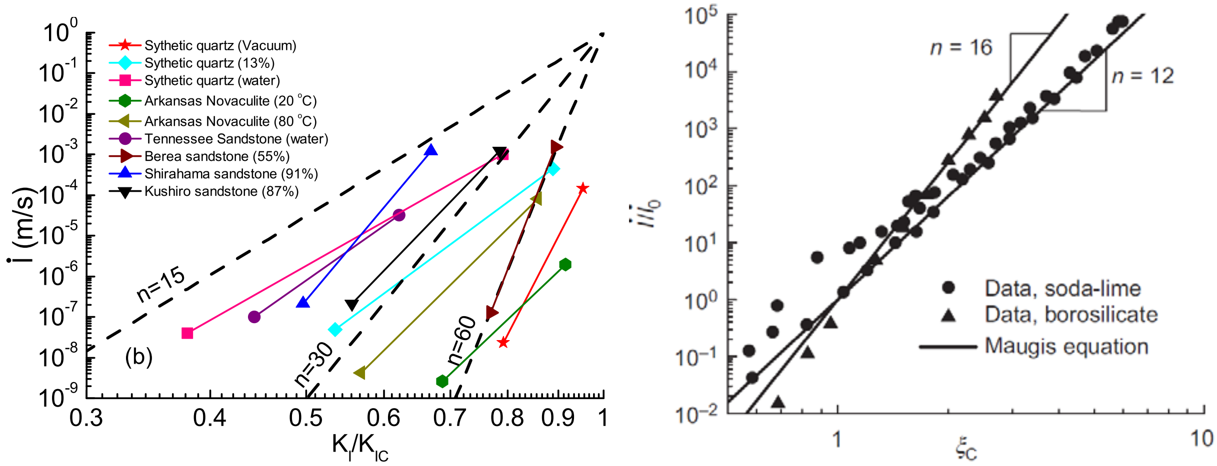


Figure 9. a) typical diagrams of the relation between crack growth velocity and stress intensity factor for various quartz-rich rocks and rock-forming minerals; b) performance of the proposed thermodynamic crack growth model.

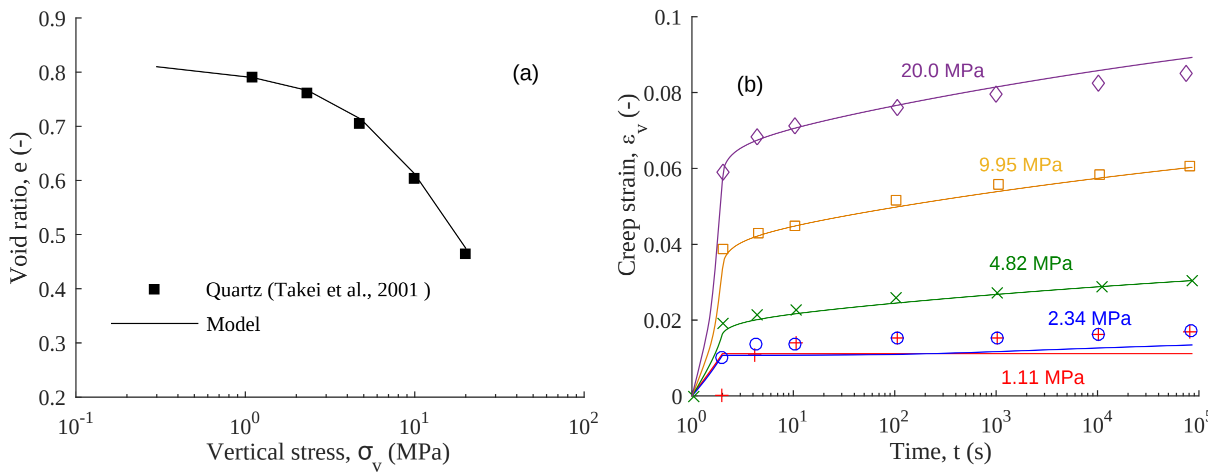


Figure 10. Comparison between creep data reported for a typical sand and the predictions of the model formulated by this project: a) compression response, b) creep response. A corrosion index within the range depicted in Figure 9a has been used to capture delayed compaction. The model captures the lack of major creep deformations at low pressures, thus corroborating the hypothesized links between yielding, delayed breakage and compression creep.

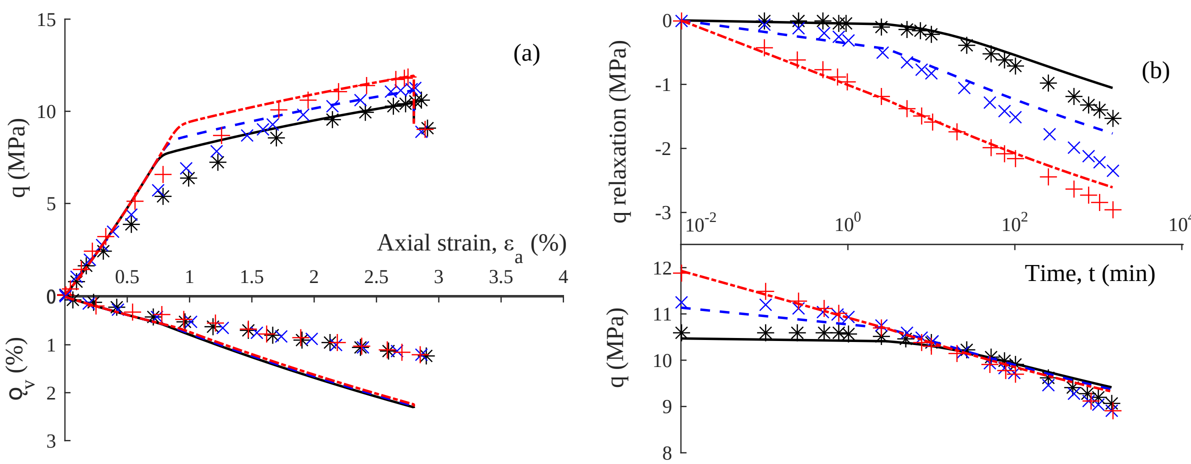


Figure 11. Experimental data and model simulations of relaxation tests on sand. The subplots show the stress-strain responses at varying rates (a) and the relative and absolute drops of stress deviator due to relaxation (b).

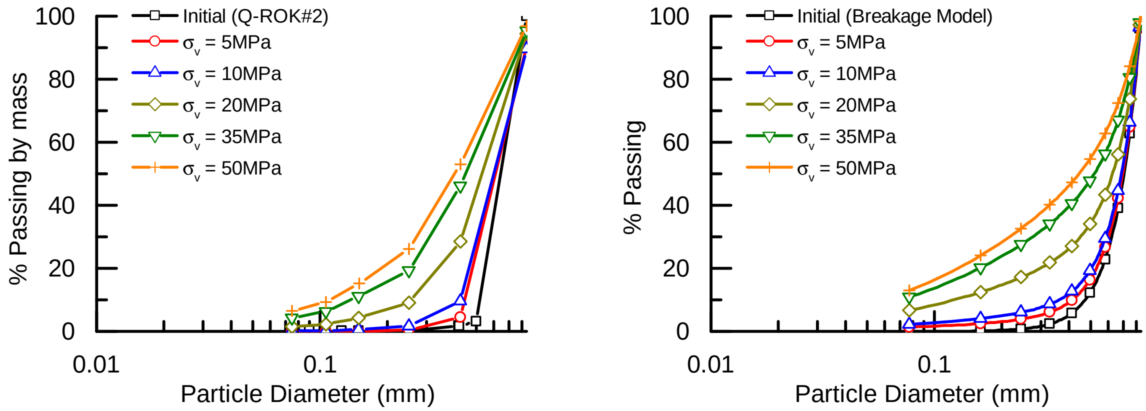


Figure 12. Measured (a) and computed (b) grain size distributions for a quartz sand subjected to varying stress state under oedometric loading. The figure illustrates the transition from a uniform gradation to a highly non-uniform state. It also shows the ability of the model to capture realistically the evolution of the degree of polydispersity.

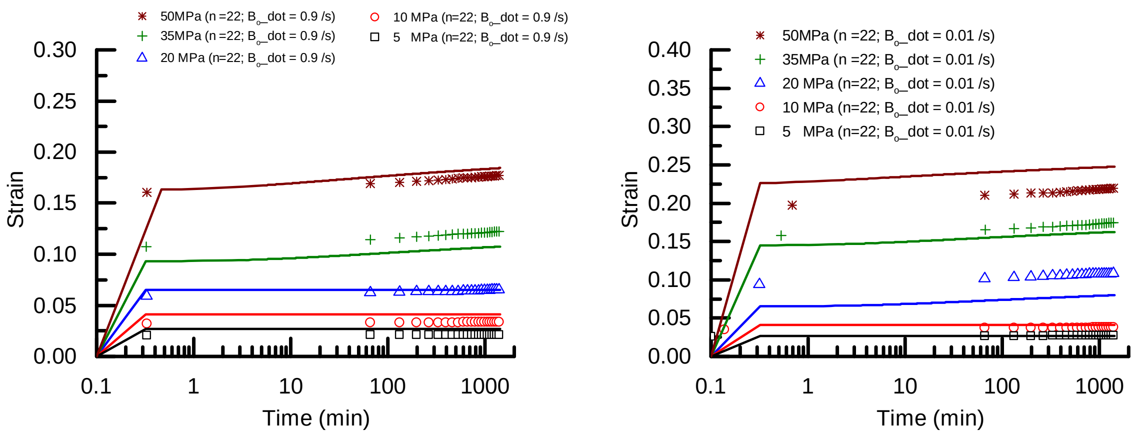


Figure 13. Measured and computed creep strains for two quartz sands subjected to axial states of stress ranging from 5 MPa to 50 MPa under oedometric conditions: (a) Q-ROK #1 (d_p = 0.350 mm); (b) Q-ROK #2 (d_p = 0.670 mm). This stage of model calibration has allowed the quantification of the grain size dependence of the parameters that control the rate-sensitivity of the granular continuum.

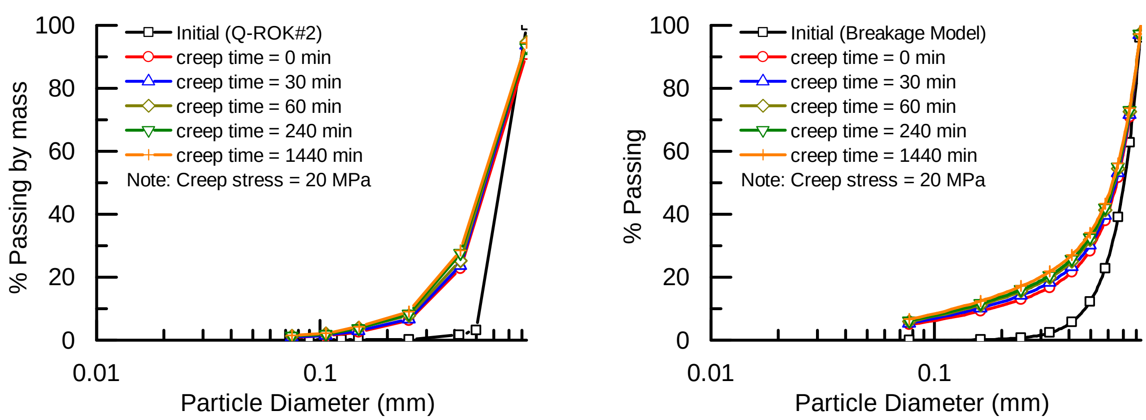


Figure 14. Example of comparison between measured (a) and computed (b) grain size distributions for a quartz sand subjected to creep. The figure shows the alteration of the degree of polydispersity as a function of time, as well as the ability of the calibrated model to capture realistically both magnitude and rate of delayed breakage.

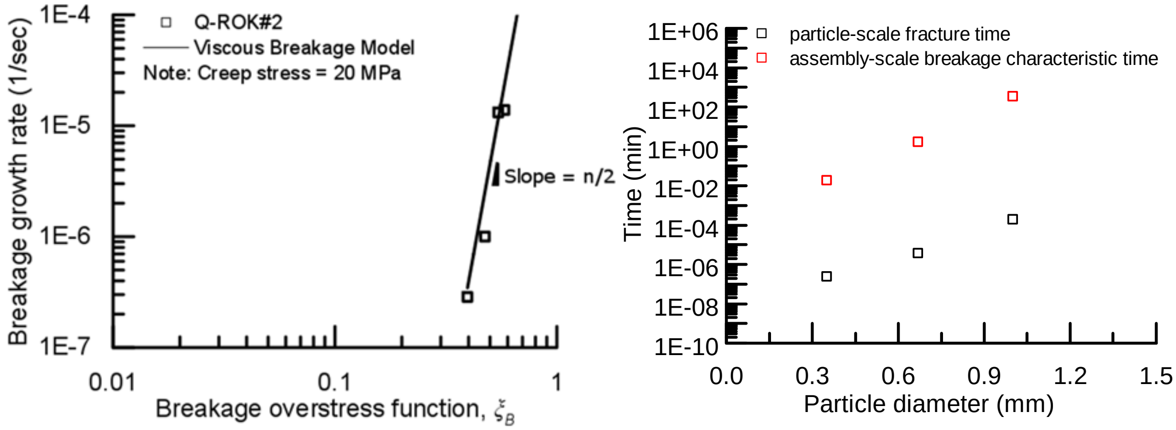


Figure 15. (a) Theoretical interpretation of the dependence between measured breakage growth rates for Q-ROK sand #2 (d_p = 0.670 mm) and the breakage overstress function (i.e., a continuum measure of the elastic energy stored in the granular system which can be released upon an incremental change of grain size distribution). The analysis illustrates the excellent performance of the proposed power law rate-dependent model based on thermodynamic considerations. Most notably, this result establishes a robust analogy between widely accepted crack growth models used to study individual subcritical fracture processes (e.g., those depicted in Figure 9 of this document). The result in Figure 15a also provides a way to assess the value of the corrosion index of the particles constituting the tested granular continuum (which in this case is n=22, a value well within the range of variability in Figure 9a). It is worth noting that this result is obtained through a single creep experiment on a packed assembly, which, by mobilizing delayed fracture in a large set of particles, guarantees statistical averaging without the need of performing numerous fracture tests on individual grains; (b) Comparison between the characteristic time of delayed comminution emerging from the model calibrations in Figure 13b and the characteristic time of failure in single particles predicted by the delayed fracture model in Figure 9b. These results suggest a remarkable consistency between the grain size dependence of particle-scale and continuum-scale quantities which can be exploited to generate robust conclusions about the relationship between the timescale of local particle failure and that of macroscopic rate-dependent deformation in granular continua under high pressures.